Wave function for no-core effective interaction approaches

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In this paper we study the method of effective interaction as it is currently applied to few-body nuclear systems, i.e., the no-core approach. We have demonstrated that in the limit of very large model space, the no-core effective Hamiltonian is equivalent to the bare Hamiltonian transformed by a unitary transformation. This result is exact to second order in the norm of the two-body Lee-Suzuki similarity transformation operator. Using this result we propose a relation between the effective *A*-body wave function and the bare wave function. Verifying this proposition through numerical calculations we have found that the resulting wave function is a rather good approximation.

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I. INTRODUCTION

In nuclear few-body problems, where one typically encounters hard-core potentials, an attempt to expand the wave function in the harmonic-oscillator (HO) or hypersphericalharmonics (HH) basis functions usually results in notoriously slow convergence. As a consequence one is either forced to introduce a correlation function into the wave function or to replace the bare interaction by an effective one, tailored to the truncated model space [1,2]. Theoretically, for a given model space one can find an effective interaction such that the low-energy spectra of the effective A-body Hamiltonian will coincide with the spectra of the full space, bare Hamiltonian [3,4]. In practice, however, finding such an effective interaction is as difficult as solving the full A-body problem. Therefore, one resorts to an approximated effective interaction, usually obtained from the solution of a two-body Hamiltonian. These two-body effective interactions no longer lead to the exact spectra in the truncated space, but if constructed properly they retain two important properties.

(i) They converge to the bare Hamiltonian if the model space is enlarged up to the full Hilbert space.

(ii) The energy levels of the effective Hamiltonian converge to the exact values faster than those of the bare Hamiltonian.

Although the advantage of this approach is evident through its recent success in nuclear few-body physics [1,2], it has two major drawbacks: the effective wave function is rather remote from the bare one, and the relation between the two is obscure. Thus, a decent interpretation of the bare wave function is missing. For closed shell nuclei these points were addressed already 40 years ago, see, for example, Refs. [5,6], and led to the development of the effective operator theory. In contrast, for no-core nuclei and for the no-core effective interaction approach no parallel treatment exist.

In the current formulation of the no-core approach the effective A-body potential is approximated by a sum of effective two-body (or three-body) potentials obtained, through the Lee-Suzuki unitary transformation method [3,4], from the solution of a two-body (three-body) Hamiltonian. Limiting our discussion to effective two-body forces, we wish to

address the following questions: Under what conditions does this approximated effective potential become exact? Alternatively, is there a unitary operator that transforms the bare *A*-body Hamiltonian into the no-core effective one?

At first sight it seems that any unitary transformation of the bare Hamiltonian will lead to a many-body, rather than a two-body, effective interaction. Consequently, the equivalence between the bare and the no-core effective Hamiltonians can be established only when the model space coincides with the full Hilbert space.

A more refined answer to the above questions can be obtained if we study the limit of very large model space. Due to property (i) any unitary transformation, connecting the bare and effective Hamiltonians, becomes unity in this limit. Moreover, the deviation of the transformation from unity can serve as a small parameter. Using these observations, we propose a form for the transformation operator and show that in the transformed Hamiltonian many-body terms fall off much faster than the two-body effective interaction terms. The resulting effective Hamiltonian coincides with the nocore one. This result holds true to second order in the small parameter.

Using this insight we attempt to bridge the gap between the effective and the bare wave functions, and propose an approximated wave function for the bare Hamiltonian. This approximation was tested numerically for the effectiveinteraction hyperspherical-harmonics (EIHH) method [2], giving rather good results.

The paper is organized as follows. In Sec. II, we review the general features common to the different no-core effective interaction methods currently used in few-body nuclear physics. In Sec. III, we study the limit of very large model space and introduce a unitary transformation operator which makes the effective and bare Hamiltonians equivalent to second order, in this limit. This transformation operator is then used to propose a relation between the bare and effective wave functions. In Sec. IV we test the quality of the wavefunction ansatz proposed in Sec. III; in order to do so we outline the calculation of mean values in the EIHH framework, and apply it to the expectation values of three-body, four-body Hamiltonians. Conclusions are given in Sec. V.

II. OUTLINE OF THE NO-CORE EFFECTIVE INTERACTION METHOD

In the effective interaction approach [1,2,7] the lowest eigenvalues of an *A*-body Hamiltonian,

$$H^{[A]} = H_0 + V \tag{1}$$

are treated as follows. The Hilbert space of $H^{[A]}$ is divided into a model space and a residual space, through the use of the eigenprojectors P and Q of H_0 , which satisfy the relations

$$[H_0, P] = [H_0, Q] = 0, \quad QH_0P = PH_0Q = 0, \quad P+Q = 1.$$
(2)

The Hamiltonian eigenvalue problem

$$H^{[A]}\Psi_{\mu} = E_{\mu}\Psi_{\mu} \tag{3}$$

is then replaced by an effective, non-Hermitian, one

$$\widetilde{H}^{[A]eff}\widetilde{\Phi}_{\mu} = (PH_0P + P\widetilde{V}^{[A]eff}P)\widetilde{\Phi}_{\mu} = E_{\mu}^{eff}\widetilde{\Phi}_{\mu}$$
(4)

that by construction has the following characteristics.

It has the same energy levels as the low-lying states of $H^{[A]}$, i.e., $E^{eff}_{\mu} = E_{\mu}$.

The effective wave functions $\tilde{\Phi}_{\mu}$ of these states are the *P*-space components of the corresponding wave function, i.e., $\tilde{\Phi}_{\mu} = P\Psi_{\mu}$.

In the Lee-Suzuki approach [3], $\tilde{H}^{[A]eff}$ is constructed through the transformation

$$\widetilde{H}^{[A]eff} = PH_0P + PVQ\omega^{[A]}P, \qquad (5)$$

where the similarity transformation operator

$$\omega^{[A]} = Q \omega^{[A]} P \tag{6}$$

fulfills the following equations:

$$\Psi_{\mu} = (P + Q\omega^{[A]}P)\tilde{\Phi}_{\mu} \tag{7}$$

for all the *P*-space energy levels $\mu = 1, ..., \dim(P)$. An equivalent *Hermitian* effective Hamiltonian can be constructed through the transformation [4]

$$H^{[A]eff} = P(H_0 + V^{[A]eff})P$$

$$= \frac{P + \omega^{[A]\dagger}}{\sqrt{P(1 + \omega^{[A]\dagger}\omega^{[A]})P}} H^{[A]} \frac{P + \omega^{[A]}}{\sqrt{P(1 + \omega^{[A]\dagger}\omega^{[A]})P}}.$$
(8)

The similarity transformation operator is the same for Eqs. (5) and (8). The Hermitian analog of the relation, Eq. (7), is

$$\Psi_{\mu} = \frac{P + \omega^{[A]}}{\sqrt{P(1 + \omega^{[A]\dagger} \omega^{[A]})P}} \Phi_{\mu}, \qquad (9)$$

where Φ_{μ} is the solution of the *Hermitian* effective Hamiltonian, i.e., $H^{[A]eff}\Phi_{\mu}=E_{\mu}\Phi_{\mu}$. In general the effective interaction appearing in Eq. (8) is an A-body interaction. Its construction is as difficult as finding the full-space solutions. Therefore, one has to approximate $V^{[A]eff}$. However,

one must build the approximate effective potential in such a way that it coincides with the bare one for $P \rightarrow 1$, so an enlargement of the model space leads to a convergence of the eigenenergies to the *true* values. The no-core shell model (NCSM) [1] and the EIHH methods are developed along these lines. In the simplest approximation $V^{[A]eff}$ is replaced by a sum of *two-body* terms

$$V^{[A]eff} \simeq \sum_{i < j}^{A} v_{ij}^{[2]eff}.$$
 (10)

The effective two-body interaction, $v_{ij}^{[2]eff}$, is derived from a "two-body" Hamiltonian

$$H_{ij}^{[2]} = H_0 + v_{ij}^{[2]}.$$
 (11)

This Hamiltonian is easily diagonalized, and the corresponding two-body similarity transformation operator, $\omega_{ij}^{[2]}$, is calculated using the appropriate analog of Eq. (7). One proceeds applying the Lee-Suzuki [4] similarity transformation to $H_{ij}^{[2]}$ in order to get the corresponding Hermitian effective Hamiltonian,

$$H_{ij}^{[2]eff} = \frac{P + \omega_{ij}^{[2]\dagger}}{\sqrt{P(1 + \omega_{ij}^{[2]\dagger}\omega_{ij}^{[2]})P}} H_{ij}^{[2]} \frac{P + \omega_{ij}^{[2]}}{\sqrt{P(1 + \omega_{ij}^{[2]\dagger}\omega_{ij}^{[2]})P}}.$$
(12)

The effective two-body potential is obtained by subtraction of H_0 ,

$$v_{ij}^{[2]eff} = \frac{P + \omega_{ij}^{[2]\dagger}}{\sqrt{P(1 + \omega_{ij}^{[2]\dagger}\omega_{ij}^{[2]})P}} H_{ij}^{[2]} \frac{P + \omega_{ij}^{[2]}}{\sqrt{P(1 + \omega_{ij}^{[2]\dagger}\omega_{ij}^{[2]})P}} - PH_0P.$$
(13)

The resulting effective Hamiltonian,

$$H^{[A]eff} \simeq H_0 + \sum_{ij} v_{ij}^{[2]eff}$$
 (14)

turns out to be an extremely good approximation as its eigenvalues converge rapidly when the *P* space is enlarged. On the other hand, using the two-body approximation of Eq. (10) one gives up rigor. As a consequence, the relation between the bare eigenstates and the effective ones, Eq. (9), does not hold any more. Moreover, even the simple interpretation of the effective wave function Φ_{μ} as the *P*-space component of the full wave function Ψ_{μ} is questionable. For obvious reasons the knowledge of the bare wave functions is very important. It is therefore desirable to restore, at least approximately, the fundamental relation of Eq. (9).

III. THE LIMIT OF VERY LARGE MODEL SPACE

Trying to find the conditions under which the approximated no-core effective potential becomes exact, lead us to seek a unitary transformation of the bare Hamiltonian, $H \rightarrow U^{\dagger}HU$, where U is chosen in a way that the P-space part of $U^{\dagger}HU$ coincides with our effective Hamiltonian, Eq. (14). When the model space coincides with the full Hilbert space then, by construction, $H^{[A]eff} = H^{[A]}$ and one can use the unit operator U=1 for such transformation. For smaller model space P < 1, and the transformation operator U deviates from unity. Hence, the question we wish to address is, to what order in this deviation does the relation $H^{[A]eff}$ $=PU^{\dagger}H^{[A]}UP$ hold true?

We start our analysis by an educated guess for the unitary transformation operator U. Considering that our attention is restricted to the P-space part of the transformed Hamiltonian, we can set the condition UQ=0. Next, we must take into account that the two-body transformation operators, $\omega_{ij}^{[2]}$, are the building blocks of our effective theory. There-fore, one might try to construct U through a power series in these operators,

$$U = P + \sum_{ij}^{A} f_{ij}^{(1)} \omega_{ij}^{[2]} + \sum_{ij,kl}^{A} g_{ij,kl}^{(2)} \omega_{kl}^{[2]\dagger} \omega_{ij}^{[2]} + \sum_{ij,kl,mn}^{A} f_{ij,kl,mn}^{(3)} \omega_{mn}^{[2]} \omega_{kl}^{[2]\dagger} \omega_{ij}^{[2]} + \cdots .$$
(15)

The condition $\omega_{ij}^{[2]} = Q \omega_{ij}^{[2]} P$ limits this expansion, and one may collect similar terms to obtain

$$U = P + g(P\omega_{mn}^{[2]\dagger}\omega_{kl}^{[2]}P) + \sum_{ij}^{A} \omega_{ij}^{[2]}f_{ij}(P\omega_{mn}^{[2]\dagger}\omega_{kl}^{[2]}P), \quad (16)$$

where g, f are functions of the *P*-space operators $P\omega_{mn}^{[2]\dagger}\omega_{kl}^{[2]}P$. It should be noted that the above expansion is rather restricted as only two particles are excited outside the P space at a time. This is an immediate consequence of the condition that the two-body similarity transformation operator, $\omega_{ii}^{[2]}$, connects the A-body P and Q spaces. This condition holds true for any state dependent effective interaction, and in particular for the EIHH method. Leaving the general discussion, we note that the starting point for the Lee-Suzuki similarity transformation [3,4] is the operator $G = \exp(\omega^{[A]})$. Introducing the approximation $\omega^{[A]} \approx \sum_{ij} \omega_{ij}^{[2]}$ into the definition of G we get,

$$G = \exp\left(\sum_{k>l=1}^{A} \omega_{kl}^{[2]}\right) = P + \sum_{k>l=1}^{A} \omega_{kl}^{[2]}.$$
 (17)

It is evident that G is not a unitary operator; moreover $G^{\dagger}G \neq P$. A transformation operator that fulfills this closure relation is given by

$$U = G \frac{1}{\sqrt{G^{\dagger}G}} = \left(P + \sum_{kl} \omega_{kl}^{[2]}\right) \frac{1}{\sqrt{P(1 + \sum_{ij,kl} \omega_{ij}^{[2]\dagger} \omega_{kl}^{[2]})P}},$$
(18)

which is our choice for the transformation operator. With this choice we can define an Hermitian effective Hamiltonian,

$$\mathcal{H}^{[A]} = U^{\dagger} H^{[A]} U$$

$$= \frac{(P + \sum_{kl} \omega_{kl}^{[2]\dagger})}{\sqrt{P(1 + \sum_{ij,kl} \omega_{ij}^{[2]\dagger} \omega_{kl}^{[2]})P}} H^{[A]}$$

$$\times \frac{(P + \sum_{mn} \omega_{mn}^{[2]})}{\sqrt{P(1 + \sum_{ij,kl} \omega_{ij}^{[2]\dagger} \omega_{kl}^{[2]})P}}.$$
(19)

The above transformation would not reproduce our effective Hamiltonian $H_{eff}^{[A]}$, Eq. (14), since $\mathcal{H}^{[A]}$ contains not only two-body terms but also three, four, and other many-body terms. The question is under what conditions do the two Hamiltonians coincide. In order to answer this question we now turn to the $P \rightarrow 1$ limit. In this limit one can assume the following.

- (i) The operators ω_{ij}^[2] are very small, ||P||≥ ||ω_{ij}^{[2]†}ω_{ij}^[2]||.
 (ii) The *Q*-space overlap between two different pairs is small with respect to same pair overlap, i.e., $\|\omega_{ii}^{[2]\dagger}\omega_{ii}^{[2]}\|$ $\gg \left\| \omega_{ij}^{[2]\dagger} \omega_{kl}^{[2]} \right\| \text{ for } (kl) \neq (ij).$

(iii) For different pairs $(ij) \neq (kl)$ the commutator be-tween the two-body interaction $v_{ij}^{[2]}$ and $\omega_{kl}^{[2]}$ is negligible, i.e., $P\omega_{ij}^{[2]\dagger}v_{kl}^{[2]} \omega_{mn}^{[2]}P \approx P\omega_{ij}^{[2]\dagger}\omega_{mn}^{[2]}v_{kl}^{[2]}P$. With these observations we see that, retaining only qua-

dratic terms in $\omega^{[2]}$,

$$\mathcal{H}_{0}^{[A]} = U^{\dagger} H_{0} U$$

$$\approx \left(P - \frac{1}{2} \sum_{ij} \omega_{ij}^{[2]^{\dagger}} \omega_{ij}^{[2]} \right) \left(P + \sum_{kl} \omega_{kl}^{[2]^{\dagger}} \right) H_{0} \left(P + \sum_{pq} \omega_{pq}^{[2]} \right) \left(P - \frac{1}{2} \sum_{rs} \omega_{rs}^{[2]^{\dagger}} \omega_{rs}^{[2]} \right) \right)$$

$$\approx \left(P - \frac{1}{2} \sum_{ij} \omega_{ij}^{[2]^{\dagger}} \omega_{ij}^{[2]} \right) \left(P H_{0} P + \sum_{kl} \omega_{kl}^{[2]^{\dagger}} H_{0} \omega_{kl}^{[2]} \right) \left(P - \frac{1}{2} \sum_{rs} \omega_{rs}^{[2]^{\dagger}} \omega_{rs}^{[2]} \right) \right)$$

$$\approx P H_{0} P + \sum_{ij} \left(\omega_{ij}^{[2]^{\dagger}} H_{0} \omega_{ij}^{[2]} - \frac{1}{2} \omega_{ij}^{[2]^{\dagger}} \omega_{ij}^{[2]} H_{0} P - \frac{1}{2} P H_{0} \omega_{ij}^{[2]^{\dagger}} \omega_{ij}^{[2]} \right)$$

$$\approx P H_{0} P + \sum_{ij} \left(\frac{P + \omega_{ij}^{[2]^{\dagger}}}{\sqrt{P(1 + \omega_{ij}^{[2]^{\dagger}} \omega_{ij}^{[2]})P}} H_{0} \frac{P + \omega_{ij}^{[2]^{\dagger}}}{\sqrt{P(1 + \omega_{ij}^{[2]^{\dagger}} \omega_{ij}^{[2]})P}} - P H_{0} P \right), \qquad (20)$$

and

$$\mathcal{V}^{[A]} = \sum_{ij} U^{\dagger} v_{ij}^{[2]} U$$

$$\approx \sum_{ij} \left(P - \frac{1}{2} \sum_{pq} \omega_{pq}^{[2]\dagger} \omega_{pq}^{[2]} \right) \left(P + \sum_{kl} \omega_{kl}^{[2]\dagger} \right) v_{ij}^{[2]} \left(P + \sum_{mn} \omega_{mn}^{[2]} \right) \left(P - \frac{1}{2} \sum_{rs} \omega_{rs}^{[2]\dagger} \omega_{rs}^{[2]} \right) \right)$$

$$\approx \sum_{ij} \left(P - \frac{1}{2} \sum_{pq} \omega_{pq}^{[2]\dagger} \omega_{pq}^{[2]} \right) \left(\sum_{(kl) \neq (ij)} \omega_{kl}^{[2]\dagger} \omega_{kl}^{[2]} v_{ij}^{[2]} + (P + \omega_{ij}^{[2]\dagger}) v_{ij}^{[2]} (P + \omega_{ij}^{[2]}) \right) \left(P - \frac{1}{2} \sum_{rs} \omega_{rs}^{[2]\dagger} \omega_{rs}^{[2]\dagger} \right) \right)$$

$$\approx \sum_{ij} \left(P - \frac{1}{2} \omega_{ij}^{[2]\dagger} \omega_{ij}^{[2]} \right) (P + \omega_{ij}^{[2]\dagger}) v_{ij}^{[2]} (P + \omega_{ij}^{[2]}) \left(P - \frac{1}{2} \omega_{ij}^{[2]\dagger} \omega_{ij}^{[2]} \right) \right)$$

$$\approx \sum_{ij} \frac{P + \omega_{ij}^{[2]\dagger}}{\sqrt{P(1 + \omega_{ij}^{[2]\dagger} \omega_{ij}^{[2]}) P}} v_{ij}^{[2]} \frac{P + \omega_{ij}^{[2]}}{\sqrt{P(1 + \omega_{ij}^{[2]\dagger} \omega_{ij}^{[2]}) P}}.$$
(21)

Combining these two results, Eqs. (20) and (21), we find that

$$\mathcal{H}^{[A]} = \mathcal{H}_{0}^{[A]} + \mathcal{V}^{[A]}$$

$$\approx PH_{0}P + \sum_{ij} \left(\frac{P + \omega_{ij}^{[2]\dagger}}{\sqrt{P(1 + \omega_{ij}^{[2]\dagger}\omega_{ij}^{[2]})P}} (H_{0} + v_{ij}^{[2]}) \right)$$

$$\times \frac{P + \omega_{ij}^{[2]}}{\sqrt{P(1 + \omega_{ij}^{[2]\dagger}\omega_{ij}^{[2]})P}} - PH_{0}P \right).$$
(22)

Thus, we can see that if our assumptions hold true, our approximated Hamiltonian of Eq. (19) coincides with the Effective Hamiltonian, Eq. (14), in the limit $P \rightarrow 1$. Of course, it is by construction that for P=1 the bare Hamiltonian and the effective one should coincide. However, this construction is not sufficient to ensure that many-body terms fall off much faster than the effective corrections to the two-body interaction. The fact that the effective Hamiltonian is exact to second order in $\omega^{[2]}$ is nontrivial. Having crossed this bridge we achieved two goals: first, we have established theoretical justification for the two-body approximation, and second, by inverting this argument we expect that Ψ_{μ} $\approx U\Phi_{\mu}$. In Sec. III A we shall elaborate on this point and discuss some further simplifications for the wave function.

Considering now the validity of our assumptions, it is evident that assumption (i) is justified. For translational invariant basis functions, i.e. basis functions that are formulated in the center of mass free (Jacobi) coordinate system, it is difficult to present a general argument in support of assumption (ii). Therefore, we shall consider this point in Sec. III B, through the specific example of the HH formalism. For single-particle states the situation is somewhat simpler. In Sec. III C, we shall discuss the validity of assumptions (ii) and (iii) using single-particle plane-wave basis functions.

A. The wave-function ansatz

Having demonstrated that in the limit $P \rightarrow 1$ the effective Hamiltonian, Eq. (14), can be obtained through a unitary transformation U, one would expect that the bare wave function can be derived from the effective one through the relation

$$|\Psi_{\mu}\rangle \approx \frac{G}{\sqrt{G^{\dagger}G}}|\Phi_{\mu}\rangle.$$
 (23)

In the following we wish to check the quality of this ansatz through numerical evaluation of the Hamiltonian expectation value for the ground-state wave function. Before we proceed, one should note that many-body operators such as $1/\sqrt{G^{\dagger}G}$ are extremely difficult to evaluate. In the transformation

$$H^{[A]} \to \frac{1}{\sqrt{G^{\dagger}G}} G^{\dagger} H^{[A]} G \frac{1}{\sqrt{G^{\dagger}G}}, \qquad (24)$$

the main role of the operator $1/\sqrt{G^{\dagger}G}$ is to insure the unitarity of the transformation, or to normalize the eigenstates of the Hamiltonian. If so, it may be instructive to use different normalization, this time not of $H^{[A]}$ but rather of its *eigenstates*,

$$|\tilde{\Psi}_{\mu}\rangle = \frac{1}{\sqrt{\langle \Phi_{\mu}|G^{\dagger}G|\Phi_{\mu}\rangle}}G|\Phi_{\mu}\rangle. \tag{25}$$

If we take seriously the statement that $1/\sqrt{G^{\dagger}G}$ is nothing more than normalization, then we can use Eq. (25) and assume that

$$\langle \Phi_{\mu} | \frac{1}{\sqrt{G^{\dagger}G}} G^{\dagger} H G \frac{1}{\sqrt{G^{\dagger}G}} | \Phi_{\mu} \rangle \simeq \frac{\langle \Phi_{\mu} | G^{\dagger} H G | \Phi_{\mu} \rangle}{\langle \Phi_{\mu} | G^{\dagger} G | \Phi_{\mu} \rangle}.$$
(26)

This form is very convenient for numerical integration, see Sec. IV. In the following we shall use Eq. (25) as our approximated wave function.

B. The validity of the second assumption in the HH formalism

In Sec. III above we have assumed that as $P \rightarrow 1$ the many-body terms fall off much faster than the two-body

terms in the effective Hamiltonian. In general, it might be rather complicated to prove this assumption. Nevertheless, in some particular cases it is possible to demonstrate its validity. Let us consider a system of *A* bosons and expand its wave function using a hyperspherical-harmonics basis. The first term in this expansion is the completely symmetric K_A =0 state. In most cases this state is also the dominant basis state in the wave functions of low-lying energy levels. It is, therefore, interesting to check whether our assumption holds for this case, and evaluate the ratio between its matrix elements for the two-body and many-body terms. For simplicity let us consider a coordinate system in which the (A-1)th Jacobi coordinate is

$$\vec{\eta}_{A-1} = \sqrt{\frac{1}{2}}(\vec{r}_{A-1} - \vec{r}_A).$$
 (27)

In this coordinate system all the quantum numbers but the principal hyperspherical quantum number, K_A , remain fixed upon application of a two-body operator, such as $v_{A,A-1}^{[2]}$ or $\omega_{A,A-1}^{[2]}$, to the $|K_A=0\rangle$ state. Thus, it is sufficient, for our purpose, to denote the basis functions by $|K_A\rangle$.

In order to evaluate the ratio

$$\frac{\langle K_A = 0 | \sum_{ij} \omega_{ij}^{[2]\dagger} \omega_{A,A-1}^{[2]} | K_A = 0 \rangle}{\langle K_A = 0 | \omega_{A,A-1}^{[2]\dagger} \omega_{A,A-1}^{[2]} | K_A = 0 \rangle},$$
(28)

we replace the particle pair (ij) by the pair (A,A-1) using two-particle permutations, and then insert a complete set of Q-space HH states to obtain

$$\langle 0 | \sum_{ij} \omega_{ij}^{[2]\dagger} \omega_{A,A-1}^{[2]} | 0 \rangle$$

$$= \sum_{ij} \langle 0 | (i,A)(j,A-1) \omega_{A,A-1}^{[2]\dagger}(i,A)(j,A-1) \omega_{A,A-1}^{[2]} | 0 \rangle$$

$$= \sum_{ij} \sum_{K \in Q} \langle 0 | \omega_{A,A-1}^{[2]\dagger} | K \rangle \langle K | (i,A)(j,A-1) | K \rangle \langle K | \omega_{A,A-1}^{[2]} | 0 \rangle.$$

$$(29)$$

In the second line we have used the fact that the principal hyperspherical quantum number is invariant to particle permutations. The two-body term is given by

$$\langle 0|\omega_{A,A-1}^{[2]\dagger}\omega_{A,A-1}^{[2]}|0\rangle = \sum_{K\in\mathcal{Q}} \langle 0|\omega_{A,A-1}^{[2]\dagger}|K\rangle\langle K|\omega_{A,A-1}^{[2]}|0\rangle.$$
(30)

The ratio between the two-body matrix element and the many-body matrix element depends on the magnitude of the pair interchanging matrix element $\langle K | (i,A)(j,A-1) | K \rangle$. Fortunately, as was shown by Fabre de la Ripelle [8], these matrix elements can be evaluated analytically. For two pairs with no common particle, $i, j \neq A, A-1$,

$$\langle K | (i,A)(j,A-1) | K \rangle = \frac{P_K^{(1/2,3A-8/2)}(1)}{P_K^{(1/2,3A-8/2)}(-1)}.$$
 (31)

When the pairs contain one common particle, for instance $j = A - 1, i \neq A$,



FIG. 1. The matrix element, Eq. (33), of the pair permutation sum, $\sum_{i>j=1} \langle K|(i,A)(j,A-1)|K\rangle$, as a function of the principal hyperspherical quantum number *K*, evaluated numerically for a system of three identical particles.

$$\langle K|(i,A)|K\rangle = \frac{P_K^{(1/2,3A-8/2)}(1/2)}{P_K^{(1/2,3A-8/2)}(-1)}.$$
(32)

Summing Eqs. (31) and (32) we get

$$\sum_{ij\neq A,A-1} \langle K | (i,A)(j,A-1) | K \rangle$$

$$= \left\{ 2(A-2) \frac{P_K^{(1/2,3A-8/2)}(1/2)}{P_K^{(1/2,3A-8/2)}(-1)} + \frac{(A-3)(A-4)}{2} \frac{P_K^{(1/2,3A-8/2)}(1)}{P_K^{(1/2,3A-8/2)}(-1)} \right\}.$$
(33)

Calculated values of the matrix element, Eq. (33), are given in Figs. 1–3 for three, four, and six bosons, respectively. Recalling that the corresponding value for the two-body term is $\langle K|K \rangle = 1$, we observe that Figs. 1–3 indicate that the con-



FIG. 2. The matrix element, Eq. (33), of the pair permutation sum, $\sum_{i>j=1} \langle K | (i,A)(j,A-1) | K \rangle$, as a function of the principal hyperspherical quantum number *K*, evaluated numerically for a system of four identical particles.



FIG. 3. The matrix element, Eq. (33), of the pair permutation sum, $\sum_{i>j=1} \langle K | (i,A)(j,A-1) | K \rangle$, as a function of the principal hyperspherical quantum number *K*, evaluated numerically for a system of six identical particles.

tributions of the many-body terms to the matrix elements of the leading $K_A=0$ state are indeed small and fall off very fast with increasing values of K. We conclude that our assumption holds for this example. Taking into account that a similar behavior is expected for all the HH states with small values of K_A , one would expect that this assumption should hold in general.

C. The single-particle plane-wave case

In the spirit of the preceeding section, we shall consider the validity of our second and third assumptions for singleparticle states through a specific example. For simplicity we shall choose a set of plane-wave basis functions. Ignoring internal degrees of freedom, we shall use the notation

$$|\vec{k}_1\vec{k}_2\dots\vec{k}_A\rangle$$

to denote a general *A*-body state. Our model space *P* is defined by the condition that each of the momenta $\vec{k_i}$ is contained in a sphere of radius *P*, i.e., $k_i = |\vec{k_i}| \leq P$. The *Q* space is the complementary space. In the following we shall use \vec{p} to denote model space momentum and by \vec{q} to denote momentum lying outside the *P*-space sphere. With these definitions it is clear that $\omega^{[2]}$ can either excite both particles into $k_i > P$ states or excite only one particle outside the *P*-space sphere. Using these observations it is convenient to write $\omega^{[2]}$ in the form

$$\omega_{12}^{[2]} = \sum_{\vec{p}_1 \vec{p}_2 \cdots \vec{p}_A} \sum_{\vec{q}_1' \vec{p}_2'} |\vec{q}_1' \vec{p}_2' \vec{p}_3 \cdots \vec{p}_A \rangle \omega_{\vec{q}_1' \vec{p}_2', \vec{p}_1 \vec{p}_2}^{[2](a)} \langle \vec{p}_1 \vec{p}_2 \cdots \vec{p}_A |$$

$$+ 1 \leftrightarrow 2 + \sum_{\vec{p}_1 \vec{p}_2 \cdots \vec{p}_A} \sum_{\vec{q}_1' \vec{q}_2'} |\vec{q}_1' \vec{q}_2' \vec{p}_3 \cdots \vec{p}_A \rangle \omega_{\vec{q}_1' \vec{q}_2', \vec{p}_1 \vec{p}_2}^{[2](b)}$$

$$\times \langle \vec{p}_1 \vec{p}_2 \cdots \vec{p}_A |. \qquad (34)$$

In the following we shall assume that $\omega^{[2]}$ is translationaly invariant. Subject to this condition, it is clear that if the ac-

tion of $\omega^{[2]}$ on the leading *P*-space states, $|\vec{p}_1 \cdots \vec{p}_A\rangle$; $p_i \ll P$, is to excite one particle outside the *P*-space sphere, then the other particle must acquire more or less the same momentum but in the opposite direction. Limiting, for the moment, our attention to these states we can use the following approximation

$$\omega_{12}^{[2]} \approx \omega_{12}^{[2](b)} = \sum_{\vec{p}_1 \vec{p}_2 \cdots \vec{p}_A} \sum_{\vec{q}_1' \vec{q}_2'} |\vec{q}_1' \vec{q}_2' \vec{p}_3 \cdots \vec{p}_A\rangle \omega_{\vec{q}_1' \vec{q}_2' \vec{p}_1 \vec{p}_2}^{[2](b)} \langle \vec{p}_1 \vec{p}_2 \cdots \vec{p}_A |.$$
(35)

With this result at hand it is evident that assumption (ii) holds,

$$\langle \vec{p}_{1}\vec{p}_{2}\dots\vec{p}_{A}|\omega_{ij}^{[2]\dagger}\omega_{kl}^{[2]}|\vec{p}_{1}'\vec{p}_{2}'\dots\vec{p}_{A}'\rangle \approx \langle \vec{p}_{1}\vec{p}_{2}\dots\vec{p}_{A}|\omega_{ij}^{[2](b)\dagger}\omega_{kl}^{[2](b)}|\vec{p}_{1}'\vec{p}_{2}'\dots\vec{p}_{A}'\rangle = \delta_{ij,kl}.$$
(36)

In order to verify assumption (iii) we have to consider the following matrix elements:

$$\langle \vec{p}_1 \vec{p}_2 \cdots \vec{p}_A | \omega_{ij}^{[2]\dagger} v_{kl}^{[2]} \omega_{mn}^{[2]} | \vec{p}_1' \vec{p}_2' \cdots \vec{p}_A' \rangle,$$

which we can divide into four topologically distinct terms,

$$\begin{split} A &= \langle \vec{p}_{1}\vec{p}_{2}\cdots\vec{p}_{A}| \ \omega_{12}^{[2](b)\dagger}v_{34}^{[2]} \ \omega_{12}^{[2](b)} \ |\vec{p}_{1}'\vec{p}_{2}'\cdots\vec{p}_{A}'\rangle, \\ B &= \langle \vec{p}_{1}\vec{p}_{2}\cdots\vec{p}_{A}| \ \omega_{12}^{[2](b)\dagger}v_{13}^{[2]} \ \omega_{23}^{[2](b)} \ |\vec{p}_{1}'\vec{p}_{2}'\cdots\vec{p}_{A}'\rangle, \\ C &= \langle \vec{p}_{1}\vec{p}_{2}\cdots\vec{p}_{A}| \ \omega_{12}^{[2](b)\dagger}v_{13}^{[2]} \ \omega_{12}^{[2](b)} \ |\vec{p}_{1}'\vec{p}_{2}'\cdots\vec{p}_{A}'\rangle, \\ D &= \langle \vec{p}_{1}\vec{p}_{2}\cdots\vec{p}_{A}| \ \omega_{12}^{[2](b)\dagger}v_{12}^{[2]} \ \omega_{12}^{[2](b)} \ |\vec{p}_{1}'\vec{p}_{2}'\cdots\vec{p}_{A}'\rangle. \end{split}$$
(37)

All the other matrix elements vanish due to Eq. (35). For case *A* it is trivial that assumption (iii) holds.

Now, let us consider case B,

$$B = \langle \vec{p}_{1}\vec{p}_{2}\cdots\vec{p}_{A} | \omega_{12}^{[2](b)\dagger}v_{13}^{[2]} \omega_{23}^{[2](b)} | \vec{p}_{1}'\vec{p}_{2}'\cdots\vec{p}_{A}' \rangle$$

$$= \delta_{\vec{p}_{4},\vec{p}_{4}'}\cdots\delta_{\vec{p}_{A},\vec{p}_{A}'}\sum_{\vec{q}_{1}\vec{q}_{2}\vec{q}_{3}} \omega_{\vec{q}_{1}\vec{q}_{2},\vec{p}_{1}\vec{p}_{2}}^{[2](b)*} \omega_{\vec{q}_{2}\vec{q}_{3},\vec{p}_{2}'\vec{p}_{3}'}^{[2](b)} \langle \vec{q}_{1}\vec{p}_{3} | v^{[2]} | \vec{p}_{1}'\vec{q}_{3} \rangle.$$
(38)

Since the potential depends only on the relative coordinate, the matrix element $\langle \vec{k_1} \vec{k_2} | v^{[2]} | \vec{k_1}' \vec{k_2} \rangle$ depends only on the relative momentum transfer, $\vec{k} = \frac{1}{2}(\vec{k_1} - \vec{k_2}) - \frac{1}{2}(\vec{k_1}' - \vec{k_2}')$. For central potentials,

$$\langle \vec{k}_1 \vec{k}_2 | v^{[2]} | \vec{k}_1' \vec{k}_2' \rangle = \delta(\vec{k}_1 + \vec{k}_2 - \vec{k}_1' - \vec{k}_2') \frac{1}{2\pi^2}$$

 $\times \int r^2 dr \ v^{[2]}(r) \frac{\sin kr}{kr},$ (39)

which for a hard-core potential $v^{[2]}(r) = V_0 \ \theta(a_0 - r)$ takes the explicit form

$$\langle \vec{k}_1 \vec{k}_2 | v^{[2]} | \vec{k}_1' \vec{k}_2' \rangle = \delta(\vec{k}_1 + \vec{k}_2 - \vec{k}_1' - \vec{k}_2') \frac{a_0^3 V_0}{2\pi^2} \\ \times \left(\frac{\sin ka_0}{(ka_0)^3} + \frac{\cos ka_0}{(ka_0)^2} \right).$$
(40)

The momentum transfer in case *B* is approximately given by

$$\vec{k} = \frac{1}{2}(\vec{q}_1 - \vec{p}_3) - \frac{1}{2}(\vec{p}_1' - \vec{q}_3) \approx \frac{1}{2}(\vec{q}_1 + \vec{q}_3) \approx \vec{q}_1,$$

where the last equality results from translation invariance, $\vec{q}_1 + \vec{p}_3 = \vec{p}'_1 + \vec{q}_3$. For large enough model space, $Pa_0 \ge 1$ and therefore

$$\langle \vec{q}_1 \vec{p}_3 | v^{[2]} | \vec{p}_1' \vec{q}_3 \rangle \propto \left(\frac{1}{a_0 q_1} \right)^2 \ll 1.$$
 (41)

To summarize, the contribution of case B is strongly suppressed due to the large momentum transfer.

Turning now to case C, we get

$$C = \langle \vec{p}_{1}\vec{p}_{2}\cdots\vec{p}_{A} | \omega_{12}^{[2](b)\dagger}v_{13}^{[2]} \omega_{12}^{[2](b)} | \vec{p}_{1}'\vec{p}_{2}'\cdots\vec{p}_{A}' \rangle$$

$$= \delta_{\vec{p}_{4},\vec{p}_{4}'}\cdots\delta_{\vec{p}_{A},\vec{p}_{A}'}\sum_{\vec{q}_{1}\vec{q}_{1}'\vec{q}_{2}}\omega_{\vec{q}_{1}\vec{q}_{2},\vec{p}_{1}\vec{p}_{2}}^{[2](b)*}\omega_{\vec{q}_{1}\vec{q}_{2},\vec{p}_{1}'\vec{p}_{2}'}^{[2](b)}\langle \vec{q}_{1}\vec{p}_{3} | v^{[2]} | \vec{q}_{1}'\vec{p}_{3}' \rangle.$$
(42)

Since $q_1 \ge p_3$ and $\vec{q}'_1 \ge \vec{p}'_3$ we can use momentum conservation to deduce the following approximation:

$$\vec{q}_1 + \vec{p}_3 = \vec{q}_1' + \vec{p}_3' \Longrightarrow \vec{q}_1 \approx \vec{q}_1'$$

On the other hand the $\omega^{[2](b)}$ matrix elements are zero unless $\vec{q}_1 + \vec{q}_2 = \vec{p}_1 + \vec{p}_2$ and $\vec{q}'_1 + \vec{q}_2 = \vec{p}'_1 + \vec{p}'_2$. Subtracting these equations we can deduce that $\vec{q}_1 - \vec{q}'_1 = \vec{p}_1 + \vec{p}_2 - (\vec{p}'_1 + \vec{p}'_2)$. Combining these results with the observation that

$$\langle \vec{q}_1 \vec{p}_3 | v^{[2]} | \vec{q}_1' \vec{p}_3' \rangle = \langle \vec{p}_1 + \vec{p}_2, \vec{p}_3 | v^{[2]} | \vec{p}_1' + \vec{p}_2', \vec{p}_3' \rangle,$$

we get

$$C \approx \delta_{\vec{p}_{4},\vec{p}_{4}'} \cdots \delta_{\vec{p}_{A},\vec{p}_{A}'} \sum_{\vec{q}_{1}\vec{q}_{2}} \omega_{\vec{q}_{1}\vec{q}_{2},\vec{p}_{1}\vec{p}_{2}}^{\lfloor 2\rfloor(b)*} \omega_{\vec{q}_{1}\vec{q}_{2},\vec{p}_{1}'\vec{p}_{2}'}^{\lfloor 2\rfloor(b)} \langle \vec{p}_{1} + \vec{p}_{2},\vec{p}_{3}|v^{[2]} \times |\vec{p}_{1}' + \vec{p}_{2}',\vec{p}_{3}'\rangle.$$
(43)

It is instructive to compare this matrix element with the matrix element

$$\begin{split} \langle \vec{p}_{1}\vec{p}_{2}\cdots\vec{p}_{A} | \ \omega_{12}^{[2](b)\dagger}\omega_{12}^{[2](b)}v_{13}^{[2]} | \vec{p}_{1}'\vec{p}_{2}'\cdots\vec{p}_{A}' \rangle \\ &= \delta_{\vec{p}_{4},\vec{p}_{4}'}\cdots\delta_{\vec{p}_{A},\vec{p}_{A}'}\sum_{\vec{q}_{1}\vec{q}_{2}\vec{p}_{1}''}\omega_{\vec{q}_{1}\vec{q}_{2},\vec{p}_{1}\vec{p}_{2}}\omega_{\vec{q}_{1}\vec{q}_{2},\vec{p}_{1}'\vec{p}_{2}}^{[2](b)}\langle \vec{p}_{1}''\vec{p}_{3} | v^{[2]} | \vec{p}_{1}'\vec{p}_{3}' \rangle \\ &= \delta_{\vec{p}_{4},\vec{p}_{4}'}\cdots\delta_{\vec{p}_{A},\vec{p}_{A}'}\sum_{\vec{q}_{1}\vec{q}_{2}}\omega_{\vec{q}_{1}\vec{q}_{2},\vec{p}_{1}\vec{p}_{2}}^{[2](b)*}\omega_{\vec{q}_{1}\vec{q}_{2},\vec{p}_{1}'\vec{p}_{2}}\langle \vec{p}_{1}''\vec{p}_{2}-\vec{p}_{2}')\vec{p}_{2}' \\ &\times \langle (\vec{p}_{1}+\vec{p}_{2}-\vec{p}_{2}')\vec{p}_{3} | v^{[2]} | \vec{p}_{1}'\vec{p}_{3}' \rangle \\ &= \delta_{\vec{p}_{4},\vec{p}_{4}'}\cdots\delta_{\vec{p}_{A},\vec{p}_{A}'}\sum_{\vec{q}_{1}\vec{q}_{2}}\omega_{\vec{q}_{1}\vec{q}_{2},\vec{p}_{1}\vec{p}_{2}}\omega_{\vec{q}_{1}\vec{q}_{2},(\vec{p}_{1}+\vec{p}_{2}-\vec{p}_{2}')\vec{p}_{2}'} \\ &\times \langle \vec{p}_{1}+\vec{p}_{2},\vec{p}_{3} | v^{[2]} | \vec{p}_{1}'+\vec{p}_{2}',\vec{p}_{3}' \rangle. \end{split}$$
(44)

Comparing Eq. (43) with Eq. (44) we can conclude that case *C* fulfills the third assumption.

In conclusion, we have shown that for $P \rightarrow 1$ the singleparticle plane-wave basis functions fulfill our assumptions. Assumption (ii) follows from Eq. (36). Assumption (iii) follows from the fact that all the $\omega^{[2]\dagger}v^{[2]}\omega^{[2]}$ matrix elements vanish except for cases A, B, C, and D. Of these, cases Aand C fulfill assumption (iii), B is negligible, and case D is singled out as the direct two-body term. During our discussion we have used the condition $p_i \ll P$. Of course this condition is not valid through all the P space. However, enlarging the P space we can fulfill this condition for any given state. We can, therefore, conclude that the transformed Hamiltonian converges to the effective one in a nonuniform way from the bottom of the P-space upward.

IV. EXPECTATION VALUES IN THE EIHH METHOD

One of the conclusions we have drawn in Sec. III is that it should be possible to approximate the bare wave function through Eq. (25). Here we would like to numerically assess the quality of this ansatz. Doing so, we shall abandon the general discussion and limit our attention for the HH formalism and, in particular, to the EIHH method.

In the HH formalism the Jacobi coordinates $(\vec{\eta}_j, j = 1...A - 1)$ are replaced by a hyperradial coordinate

$$\rho = \sqrt{\sum_{j=1}^{N} \vec{\eta}_j^2},\tag{45}$$

and a hyperangle Ω_A . The unperturbed Hamiltonian H_0 is chosen to be

$$H_0 = T_K(\rho) \equiv \frac{1}{2m} \frac{\hat{K}_A^2}{\rho^2},$$
(46)

the hypercentrifugal kinetic energy operator, with the hyperspherical harmonics $\mathcal{Y}_{[K_A]}$ as eigenfunctions ($[K_A]$ stands for a set of quantum numbers, see Ref. [2]). The model space *P* is defined as the complete set of HH basis functions with generalized angular momentum quantum number $K_A \leq K_P$, and the *Q* space as the complete set of HH basis functions with $K_A > K_P$. The hyperradial coordinate ρ serves as a parameter in the construction of the HH effective interaction as it commutes with $T_K(\rho)$. It should be noted that in the EIHH method $\omega_{ij}^{[2]} = \omega_{ij}^{[2]}(\rho)$. Moreover, because the HH effective interaction is state dependent, $\omega_{ij}^{[2]}$ transforms an *A*-body *P*-space state into an *A*-body *Q*-space state. The structure of $\omega_{ij}^{[2]}$ becomes simple if we choose $\tilde{\eta}_{ij} = 1/\sqrt{2}(\tilde{r_i} - \tilde{r_j})$ as the "last," (A-1), Jacobi coordinate. For such a coordinate system

$$\omega_{ij}^{[2]}(\rho) = \sum_{K_Q \in Q, K_P \in P} |[K_{A-2}]K_Q jt \rangle \omega_{K_Q, K_P}^{[K_{A-2}]jt}(\rho) \langle [K_{A-2}]K_P jt |,$$
(47)

where j, t are the angular momentum and isospin of the twoparticle system, and $[K_{A-2}]$ stands for the hypersphericalspin-isospin quantum numbers of the residual (A-2)-body system. The resulting effective Hamiltonian is written in the HH formalism as

$$H^{[A]eff} = T_{\rho} + T_{K}(\rho) + \sum_{ij} v_{ij}^{[2]eff}(\rho), \qquad (48)$$

where

$$T_{\rho} = -\frac{1}{2m} \Delta_{\rho} \tag{49}$$

is the hyperradial kinetic energy. The operator Δ_{ρ} is the Laplace operator with respect to the hyperradial coordinate ρ .

In order to diagonalize the effective Hamiltonian we expand the effective, P space, wave functions in the following way:

$$|\Phi_{\mu}\rangle = \sum_{[K_A]n} C^{\mu}_{[K_A]n} |n\rangle |[K_A]\rangle, \qquad (50)$$

where for brevity we have used the notation

$$[K_A] \equiv K_A J_A J_A^z T_A T_A^z \Gamma_A \alpha_A \beta_A$$

The antisymmetric *A*-body hyperspherical-spin-isospin basis functions with total angular momentum J_A, J_A^z and isospin $T_A T_A^z$ are given by [12–14]

$$|K_{A}J_{A}J_{A}^{z}T_{A}T_{A}^{z}\Gamma_{A}\alpha_{A}\beta_{A}\rangle = \sum_{Y_{A-1}} \frac{\Lambda_{\Gamma_{A},Y_{A-1}}}{\sqrt{|\Gamma_{A}|}} [|K_{A}L_{A}M_{A}\Gamma_{A}Y_{A-1}\alpha_{A}\rangle \\ \times |S_{A}S_{A}^{z}T_{A}T_{A}^{z}\widetilde{\Gamma_{A}},\widetilde{Y}_{A-1}\beta_{A}\rangle]^{J_{A}J_{A}^{z}},$$
(51)

where

$$\mathcal{Y}^{A}_{K_{A}L_{A}M_{A}\Gamma_{A}Y_{A-1}\alpha_{A}}(\Omega_{A}) \equiv \langle \Omega_{A} | K_{A}L_{A}M_{A}\Gamma_{A}Y_{A-1}\alpha_{A} \rangle \quad (52)$$

are HH functions with hyperspherical angular momentum $K=K_A$, and orbital angular momentum quantum numbers L_A, M_A that belong to well defined irreducible representations (irreps) $\Gamma_1 \in \Gamma_2 \cdots \in \Gamma_A$, of the permutation group-subgroup chain $S_1 \subset S_2 \cdots \subset S_A$, denoted by the Yamanouchi symbol $[\Gamma_A, Y_{A-1}] \equiv [\Gamma_A, \Gamma_{A-1}, \cdots, \Gamma_1]$. The dimension of the irrep Γ_m is denoted by $|\Gamma_m|$ and $\Lambda_{\Gamma_A, Y_{A-1}}$ is a phase factor [9]. Similarly, the function

$$\chi^{A}_{S_{A}S^{z}_{A}T_{A}T^{z}_{A}\widetilde{\Gamma}_{A},\widetilde{Y}_{A-1}\beta_{A}}(\sigma\tau) \equiv \langle \sigma\tau | S_{A}S^{z}_{A}T_{A}T^{z}_{A}\widetilde{\Gamma}_{A},\widetilde{Y}_{A-1}\beta_{A} \rangle$$
(53)

are the symmetrized spin-isospin basis functions, where the *A*-dimensional vectors $\sigma \equiv (s_1^z, s_2^z \cdots s_A^z)$ and $\tau \equiv (t_1^z, t_2^z \cdots t_A^z)$ stand for the *A*-body spin and isospin states. The quantum numbers α_A, β_A are used to remove the degeneracy of the HH and spin-isospin states, respectively. For the hyperradial basis functions, we have used the associated Laguerre polynomials, $L_n^\alpha(x)$, with range parameter *b*,

$$R_n(\rho) \equiv \langle \rho | n \rangle = \sqrt{\frac{n!}{(n+\alpha)!}} b^{-\alpha/2} \rho^{\alpha - (3A-4)/2} L_n^{\alpha}(\rho/b)$$
$$\times \exp(-\rho/2b). \tag{54}$$

Taking $\mu=0$ to be the ground state of an A body system, we find that the corresponding bare wave function is approximately given by Eq. (25),

$$\Psi_{0}(\rho,\Omega,\sigma,\tau) = \langle \rho,\Omega,\sigma,\tau | \Psi_{0} \rangle = \frac{1}{\sqrt{\mathcal{N}}} \langle \rho,\Omega,\sigma,\tau | G | \Phi_{0} \rangle$$
$$= \frac{1}{\sqrt{\mathcal{N}}} \langle \rho,\Omega,\sigma,\tau | \left(1 + \sum_{i>j=1}^{A} \omega_{ij}^{[2]}(\rho)\right) | \Phi_{0} \rangle,$$
(55)

were \mathcal{N} is the normalization constant,

$$\mathcal{N} = \langle \Phi_0 | G^{\dagger} G | \Phi_0 \rangle = \sum_{\sigma \tau} \int d\Omega d\rho \rho^{3N-1} | \langle \rho, \Omega, \sigma, \tau | G | \Phi_0 \rangle |^2.$$
(56)

In order to evaluate the quality of this wave function, we would like to evaluate its expectation value of the Hamiltonian, and see how well it reproduces the binding energy of an *A* body system. The expectation value of any local operator defined in our Hilbert space 1=P+Q is given by,

$$\langle \Psi_0 | \hat{O} | \Psi_0 \rangle = \frac{1}{\mathcal{N}} \sum_{\sigma \sigma', \tau \tau'} \int d\Omega d\rho \rho^{3N-1} \Psi_0(\rho, \Omega, \sigma, \tau)^*$$
$$\times \hat{O}_{\sigma \tau, \sigma' \tau'}(\Omega, \rho) \Psi_0(\rho, \Omega, \sigma', \tau').$$
(57)

Since in our Jacobi coordinate system of choice the "last" [i.e., (A-1)] Jacobi coordinate is proportional to the separation of particles *A* and (A-1) it is convenient to make the substitution

$$\omega_{ij}^{[2]} = (A - 1, i)(A, j)\omega_{A, A - 1}^{[2]}(A, j)(A - 1, i),$$
(58)

use the permutational symmetry of Φ_0 , and evaluate Ψ_0 in the form,

$$\Psi_0(
ho,\Omega,\sigma, au)$$

$$= \frac{1}{\sqrt{\mathcal{N}}} \langle \rho, \Omega, \sigma, \tau | \left(1 + \sum_{i>j=1}^{A} (A-1,i)(A,j)\omega_{A,A-1}^{[2]}(\rho) \right) | \Phi_0 \rangle$$

$$= \frac{1}{\sqrt{\mathcal{N}}} \left(\langle \rho, \Omega, \sigma, \tau | \Phi_0 \rangle + \sum_{i>j=1}^{A} {}_{ij} \langle \rho, \Omega, \sigma, \tau | \omega_{A,A-1}^{[2]} \right)$$

$$\times (\rho) | \Phi_0 \rangle \right).$$
(59)

In the last equation we used the notation

$$|\rho,\Omega,\sigma,\tau\rangle_{ii} = (i,A-1)(j,A)|\rho,\Omega,\sigma,\tau\rangle$$
 (60)

to denote the permutation of the space-spin-isospin configuration. The symmetrized hyperspherical-harmonics functions [13,14] are constructed through a recursive permutation of the HH "tree" functions [10]. By successive implementation of the recursive construction we get

$$K_{A}L_{A}M_{A}Y_{A}\beta_{A}\rangle$$

$$=\sum_{\ell_{A}}\sum_{\beta_{A}}\sum_{[K_{A-2}]}\prod_{i=1}^{A-2} [K_{i}L_{i}\ell_{i+1}\beta_{i}\Gamma_{i}|K_{i+1}L_{i+1}\beta_{i+1}\Gamma_{i+1}$$

$$\times [K_{A-1}L_{A-1}\Gamma_{A-1}\beta_{A-1}|K_{A}L_{A}\Gamma_{A}\beta_{A}|$$

$$\times ([K_{A-2}];\ell_{A})K_{A}L_{A}M_{A}\rangle$$

$$\equiv \sum_{[K_{A-2}],\ell_{A}\in K_{A},L_{A}}U_{[K_{A-2}],\ell_{A}}^{K_{A},L_{A},Y_{A},\beta_{A}} |([K_{A-2}];\ell_{A})K_{A}L_{A}M_{A}\rangle.$$
(61)

Here we used the notation $[K_{A-2}]$ to denote the HH tree quantum numbers and the relations $K_A = K_{A-1}, L_A = L_{A-1}$. The spin-isospin states are constructed very much the same way. After having transformed the symmetrized HH functions into tree functions and the symmetrized spin-isospin states into regular unsymmetrized states, one can use standard angular momentum techniques and evaluate $\Psi_0(\rho, \Omega, \sigma, \tau)$. The resulting expression can then be used to evaluate the expectation value, Eq. (57). In practice we have used Monte-Carlo integration with the metropolis algorithm to evaluate the spatial integral,

$$\langle \Psi_0 | \hat{O} | \Psi_0 \rangle \approx \frac{1}{N_{MC}} \sum_{i=1}^{N_{MC}} \sum_{\sigma\sigma',\tau\tau'} \Psi_0(\rho_i, \Omega_i, \sigma, \tau)^*$$
$$\times \hat{O}_{\sigma\tau,\sigma'\tau'}(\rho_i, \Omega_i) \Psi_0(\rho_i, \Omega_i, \sigma', \tau').$$
(62)

This scheme is very effective, since $|\Psi_0(\rho,\Omega,\sigma,\tau)|^2$ is the distribution probability and therefore serves as a natural weight function.

As an example we consider a system of A nucleons interacting via the simple Malfliet-Tjon [11], MTV, nucleonnucleon interaction. Numerical results for the A=3 case are presented in Table I and for the A=4 case in Table II. In these tables we study the convergence of the Hamiltonian expectation value for the ground state as a function of K_P , which fixes the size of the model space. For comparison we also present the value of the ground-state energy obtained through direct diagonalization of the bare Hamiltonian in the model space. Also presented are ground-state energies obtained by different methods. It can be seen that the proposed wave function can reproduce the binding energies of these systems to few parts per thousand, and as expected the quality of the wave function improves with enlargement of the model space.

V. CONCLUSIONS

In this paper we studied the method of the effective interaction as it is currently applied to few-body nuclear systems, i.e., all nucleons active. We have managed to demonstrate that in the limit $P \rightarrow 1$ the no-core effective Hamiltonian is equivalent through unitary transformation to the bare Hamiltonian. We have also shown that this holds true to second order in the norm of the two-body Lee-Suzuki similarity TABLE I. Ground-state energy (MeV) of three-particle system, interacting via the MTV potential. The Hamiltonian expectation value, right-side column, and the noneffective binding energy, middle column, are given as a function of the *P*-space size by the principal HH quantum number K_P . The expectation value is approximated using Eq. (26).

K_P	Noneffective	$\langle \Psi_0 H^{[A]} \Psi_0 angle$
0	0.6825	6.7020 ± 0.2637
4	2.1443	8.1970 ± 0.0891
6	4.6407	8.1735 ± 0.0428
8	5.4207	8.2134 ± 0.0242
10	6.3405	8.2442 ± 0.0203
12	7.0954	8.2197 ± 0.0226
EIHH [2]	8.244(8)	
NCSM [1]	8.235(5)	
SVM [17]	8.2527	
Faddeev [20]	8.25273	
GFMC [18]	8.26(1)	
CHH [21]	8.240	
ATMS [19]	8.26(1)	
VMC [17]	8.27(3)	

transformation operator, $\|\omega^{[2]}\|$. Using this result, we have proposed a new interpretation for the relation between the effective *A*-body wave function and the bare wave function. Verifying this proposition through numerical calculations, we have found out that the resulting wave function is a rather good approximation.

TABLE II. Ground-state energy (MeV) of four-particle system, interacting via the MTV potential. The Hamiltonian expectation value, right-side column, and the noneffective binding energy, middle column, are given as a function of the *P*-space size by the principal HH quantum number K_P . The expectation value is approximated using Eq. (26).

K _P	Noneffective	$\langle \Psi_0 {\it H}^{[A]} \Psi_0 angle$
0	7.4059	27.137±0.824
4	9.5749	30.536 ± 0.462
6	13.934	30.284 ± 0.678
8	20.500	30.911 ± 0.315
10	23.502	30.865 ± 0.302
12	26.585	31.024 ± 0.220
14	28.036	31.156 ± 0.115
16	29.163	31.287 ± 0.045
EIHH [2]	31.358(9)	
SVM [17]	31.360	
FY [20]	31.36	
ATMS [19]	31.36	
CRCG [22]	31.357	
GFMC [18]	31.3(2)	
VMC [17]	31.30(5)	

As a result, effective two-body operators constructed through the relation [15,16]

$$O_{ij}^{[2]eff} = \frac{P + \omega_{ij}^{[2]\dagger}}{\sqrt{P(1 + \omega_{ij}^{[2]\dagger}\omega_{ij}^{[2]})P}} O_{ij}^{[2]} \frac{P + \omega_{ij}^{[2]}}{\sqrt{P(1 + \omega_{ij}^{[2]\dagger}\omega_{ij}^{[2]})P}}$$
(63)

can be regarded as accurate to second order in the limit $P \rightarrow 1$. This observation opens the way to the application of the

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